

Naphazoline

835-31-4 | DTXSID3048449

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -10.4 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.46e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Methyl-p-benzoquinone

Measured: -10.6

Predicted: -10.7

[Image not found](#)

1,3,5-Cycloheptatriene

Measured: -10.0

Predicted: -10.0

[Image not found](#)

1,4-Benzoquinone

Measured: -11.3

Predicted: -11.2